MODIFICATION OF THE COULOMB INTERACTION BETWEEN ELECTRIC CHARGES OR DIPOLES IN LAYERED STRUCTURES: INFLUENCE OF MANY-BODY EFFECTS

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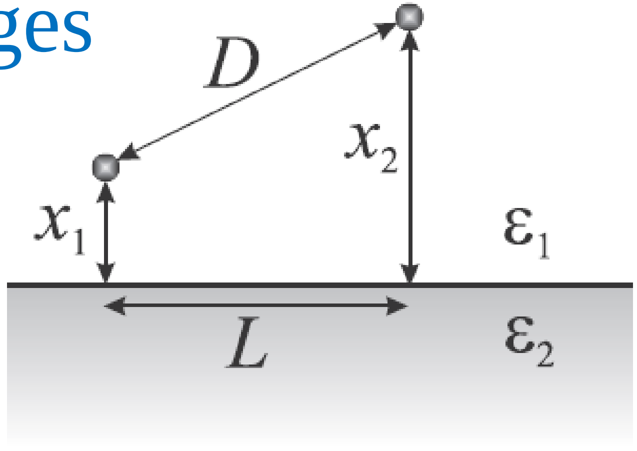
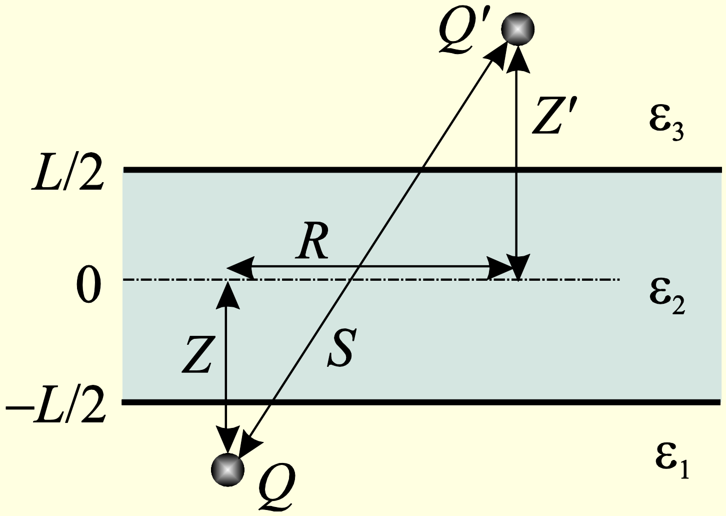
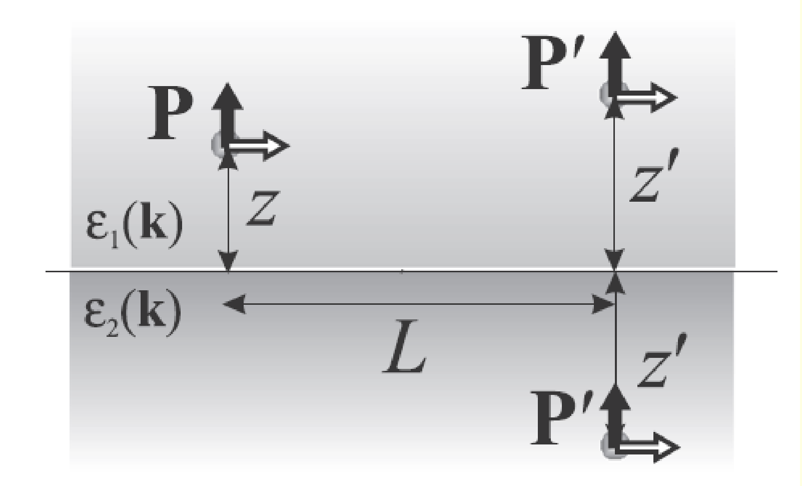
CHARGES OR DIPOLES IN TWO- AND THREE-LAYER STRUCTURES

Charges





Dipoles



WHY DO WE NEED TO KNOW ELECTROSTATIC INTERACTIONS IN LAYERED SYSTEMS?

PHYSICAL REVIEW B **84**, 045418 (2011)

Electrostatic model for treating long-range lateral interactions between polar molecules adsorbed on metal surfaces

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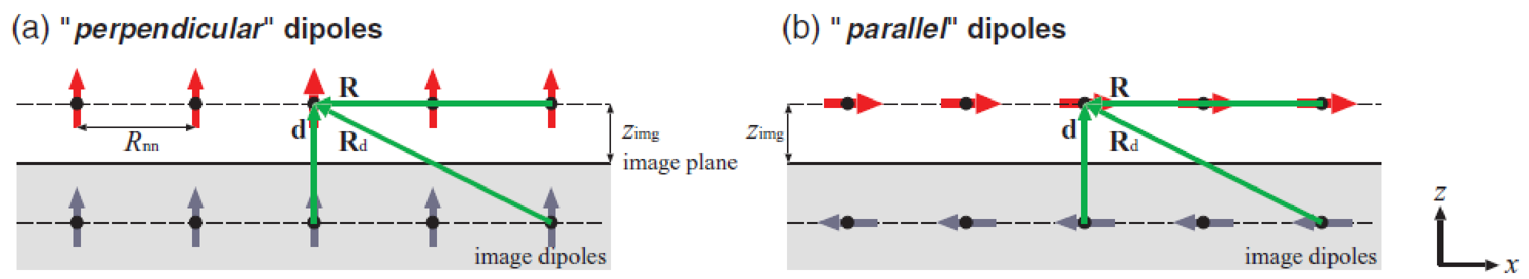
(Received 3 March 2011; revised manuscript received 13 April 2011; published 11 July 2011)



WHY DO WE NEED TO KNOW ELECTROSTATIC INTERACTIONS IN LAYERED SYSTEMS?

High-temperature electron-hole superfluidity with strong anisotropic gaps in double phosphorene monolayers

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Excitonic superfluidity in double phosphorene monolayers is investigated using the BCS mean-field equations. Highly anisotropic superfluidity is predicted where we found that the maximum superfluid gap is in the Bose-Einstein condensate (BEC) regime along the armchair direction and in the BCS-BEC crossover regime along the zigzag direction. We estimate the highest Kosterlitz-Thouless transition temperature with maximum value up to $\sim$90 K with onset carrier densities as high as 4×10^{12} cm^{-2}. This transition temperature is significantly larger than what is found in double electron-hole few-layers graphene. Our results can guide experimental research toward the realization of anisotropic condensate states in electron-hole phosphorene monolayers.

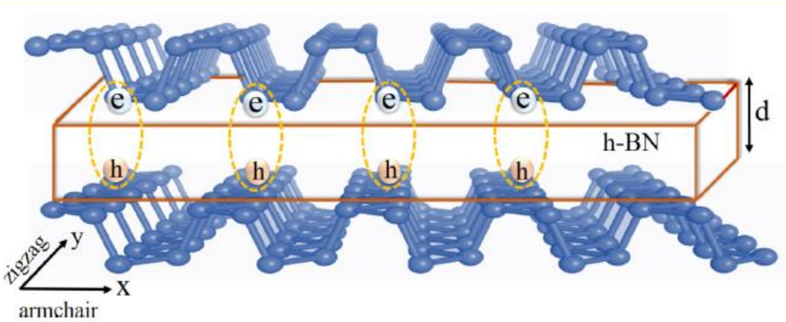

FIG. 1. Schematic illustration of two phosphorene sheets separated by a thin barrier of h-BN layers. The electrons and holes are induced by top and back gates in the separately electrically contacted upper and lower phosphorene sheets.

WHY DO WE NEED TO KNOW ELECTROSTATIC INTERACTIONS IN LAYERED SYSTEMS?

Yuriy Monarkha   Kimitoshi Kono

Two-Dimensional Coulomb Liquids and Solids

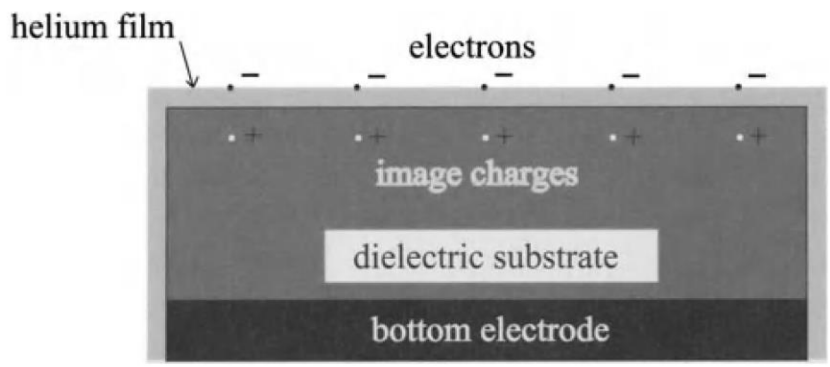

Fig. 1.7. Schematic view of SEs on a helium film and major image charges

WHY DO WE NEED TO KNOW ELECTROSTATIC INTERACTIONS IN LAYERED SYSTEMS?

Superlattices and Microstructures, Vol. 4, No. 4/5, 1988

EXCITONS AND POLARITONS IN SEMICONDUCTOR/INSULATOR QUANTUM WELLS AND SUPERLATTICES

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(Received 22 February 1988)

Schemes for increasing the binding energies of Wannier-Mott excitons in semiconductor/insulator quantum wells and superlattices are proposed.

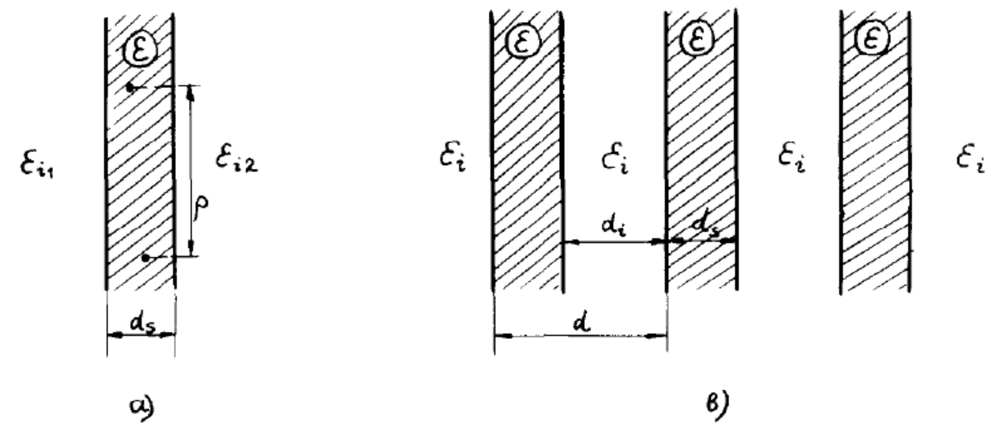

Fig. 1. Semiconductor-insulator quantum well (a) and superlattice (b).

WHY DO WE NEED TO KNOW ELECTROSTATIC INTERACTIONS IN LAYERED SYSTEMS?

PHYSICAL REVIEW B **88**, 045318 (2013)

Theory of neutral and charged excitons in monolayer transition metal dichalcogenides

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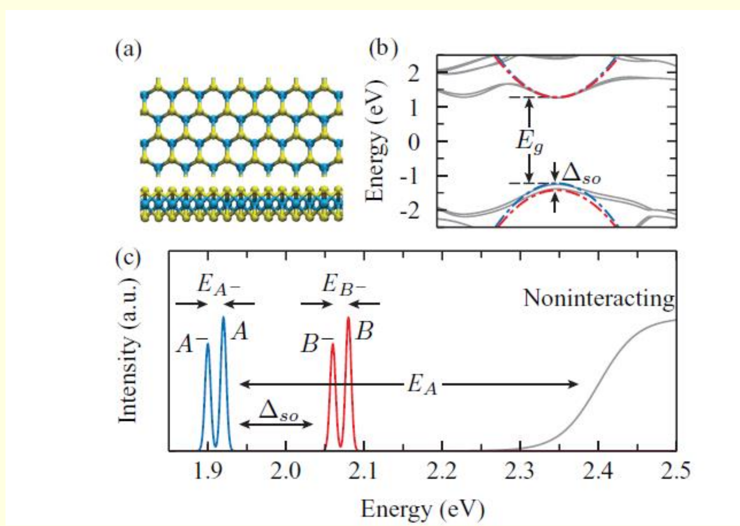
We present a microscopic theory of neutral excitons and charged excitons (trions) in monolayers of transition metal dichalcogenides, including molybdenum disulfide. Our theory is based on an effective mass model of excitons and trions, parameterized by *ab initio* calculations and incorporating a proper treatment of screening in two dimensions. The calculated exciton binding energies are in good agreement with high-level many-body computations based on the Bethe-Salpeter equation. Furthermore, our calculations for the more complex trion species compare very favorably with recent experimental measurements and provide atomistic insight into the microscopic features which determine the trion binding energy.



THEORETICAL METHOD: CLASSICAL AND NON-LOCAL ELECTROSTATICS

1 *THEORY OF CHARACTERISTIC ENERGY LOSSES IN THIN FILMS*

Yu. A. ROMANOV

J. Exptl. Theoret. Phys. (U.S.S.R.) **47**, 2119–2133 (December, 1964)

2 **Screening of charges and Friedel oscillations of the electron density in metals having differently shaped Fermi surfaces**

A. M. Gabovich, L. G. Il'chenko, E. A. Pashitskiĭ, and Yu. A. Romanov

Sov. Phys. JETP **48**(1), July 1978

3 **CHARGE INTERACTION IN LAYERED SYSTEMS WITH SPATIAL DISPERSION**

L.G. IL'CHENKO, E.A. PASHITSKII and Yu.A. ROMANOV

Surface Science 121 (1982) 375–395

4 **DYNAMICAL IMAGE FORCES IN THREE-LAYER SYSTEMS AND FIELD EMISSION**

A.M. GABOVICH, V.M. ROSENBAUM and A.I. VOITENKO

Surface Science 186 (1987) 523–549

INTERACTION AS A FUNCTIONAL OF GREEN'S FUNCTIONS

$$W_{ij}(R,Z,Z') = -2QQ' \int_0^\infty q\,dq\,D_{ij}(q,Z,Z')\,J_0(qR),$$

where the subscripts i and j denote the medium where the charges Q and Q', respectively, are located; R is the horizontal distance between the charges, Z and Z' are their vertical coordinates; and $J_0(x)$ is the Bessel function of the first kind.

Green's functions

$$D_{ij} = \frac{A_i(Z)B_j(Z') + \widetilde{A}_i(Z)\widetilde{B}_j(Z')}{C} - F_i(Z,Z')\delta_{ij},$$

$$A_1(Z) = \widetilde{A}_1(Z) = a_1(Z),$$

$$A_2(Z) = -a_S(Z), \quad \widetilde{A}_2(Z) = -a_A(Z),$$

$$A_3(Z) = -\widetilde{A}_3(Z) = a_3(Z-L),$$

$$W_{QQ'} = \frac{QQ'}{L}w$$

INTERACTION AS A FUNCTIONAL OF GREEN'S FUNCTIONS

$$B_1(Z') = a_1(Z')\left[a_A(0) + a_3(0)\right],$$
$$\widetilde{B}_1(Z') = a_1(Z')\left[a_S(0) + a_3(0)\right],$$

$$\begin{aligned} B_2(Z') = -\frac{1}{2}\{&[a_S(Z') + a_A(Z')]\left[a_A(0) + a_3(0)\right] \\ &+ [a_S(Z') - a_A(Z')]\left[a_A(0) + a_1(0)\right]\}, \end{aligned}$$
$$\begin{aligned} \widetilde{B}_2(Z') = -\frac{1}{2}\{&[a_S(Z') + a_A(Z')]\left[a_S(0) + a_3(0)\right] \\ &- [a_S(Z') - a_A(Z')]\left[a_S(0) + a_1(0)\right]\}, \end{aligned}$$

$$B_3(Z') = a_3(Z' - L)\left[a_A(0) + a_1(0)\right],$$
$$\widetilde{B}_3(Z') = a_3(Z' - L)\left[a_S(0) + a_1(0)\right],$$

$$\begin{aligned} C = &\left[a_S(0) + a_1(0)\right]\left[a_A(0) + a_3(0)\right] \\ &+ \left[a_S(0) + a_3(0)\right]\left[a_A(0) + a_1(0)\right], \end{aligned}$$

$$F_1(Z, Z') = b_1(Z, Z'),$$
$$F_2(Z, Z') = \frac{1}{2}\left[b_S(Z, Z') + b_A(Z, Z')\right],$$
$$F_3(Z, Z') = b_3(Z, Z'),$$

INTERACTION AS A FUNCTIONAL OF GREEN'S FUNCTIONS

$$a_{1,3}(Z) = \frac{1}{\pi}\int\limits_{-\infty}^{+\infty} \frac{dk_\perp \cos k_\perp Z}{(k_\perp^2 + q^2)\,\varepsilon_{1,3}(\mathbf{q}, k_\perp, \omega)},$$

$$a_{S,A}(Z) = \frac{2}{L}\sum_{k_\perp^{S,A}} \frac{\exp(ik_\perp Z)}{(k_\perp^2 + q^2)\,\varepsilon_2(\mathbf{q}, k_\perp, \omega)},$$

$$k_\perp^S = \frac{2n\pi}{L}, \quad k_\perp^A = \frac{(2n+1)\,\pi}{L} \qquad (n = 0, \pm 1, \pm 2, ..)\,,$$

$$b_1(Z, Z') = \frac{1}{2}\left\{a_1(Z + Z') + a_1(Z - Z')\right\},$$

$$b_{S,A}(Z, Z') = \frac{1}{2}\left[a_{S,A}(Z + Z') + a_{S,A}(Z - Z')\right],$$

$$b_3(Z, Z') = \frac{1}{2}\{a_3(|Z - L| + |Z' - L|)$$
$$+a_3(|Z - L| - |Z' - L|)\}\,.$$

THE OLD PROBLEM REVISITED: CHARGES. EFFECTIVE POWER EXPONENT IN A TWO-LAYER SYSTEM

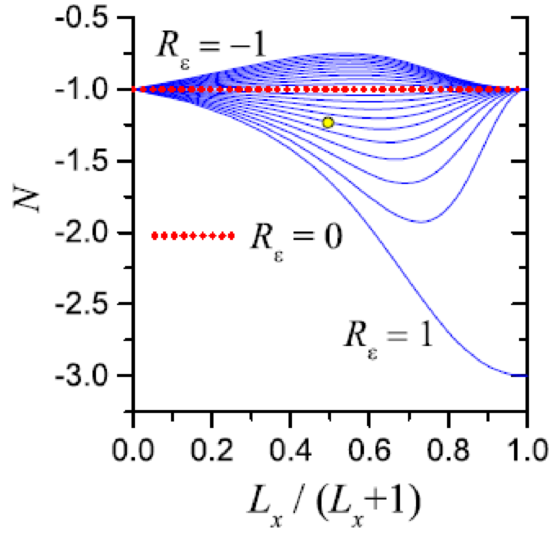


Figure 4. Dependences of the apparent value of the power exponent N in the Coulombic-like dependence (9) on the distance between the charges for various R_ε values. The R_ε step between the curves equals 0.1. The point corresponds to the point in figure 3.

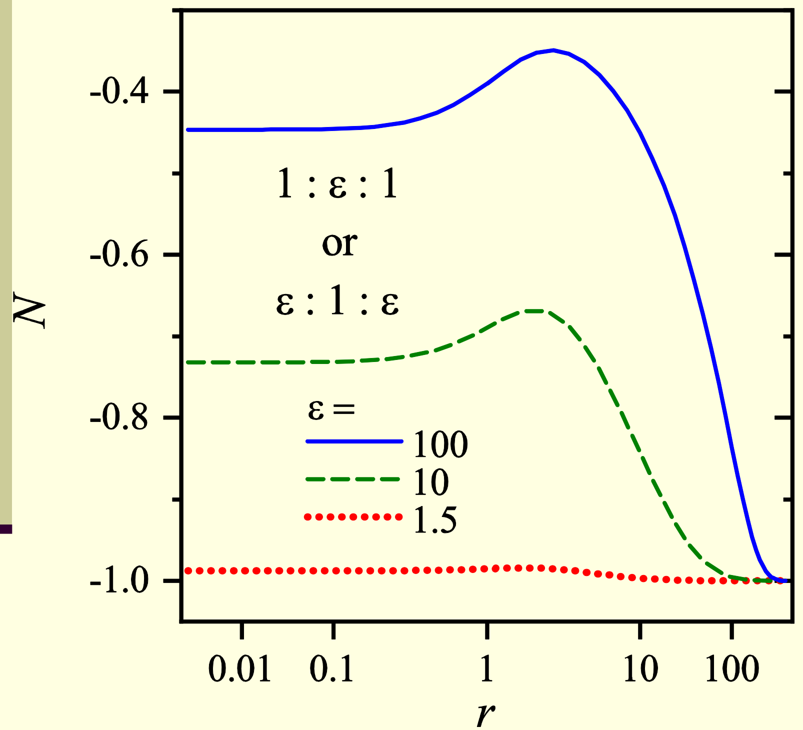
Up to the dipole-like behavior

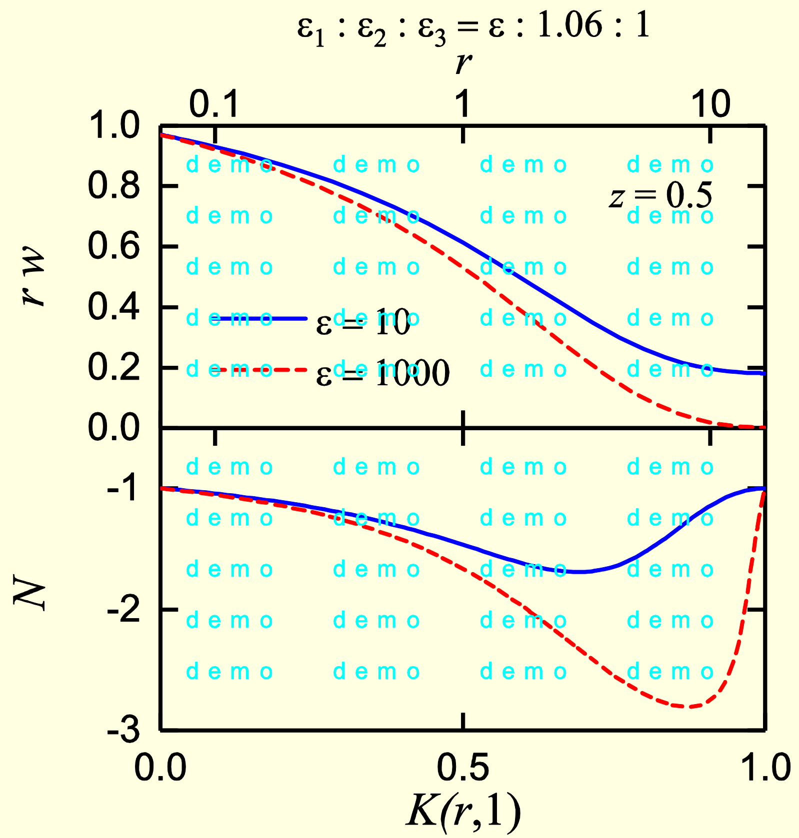
$$W \approx C_N L^N$$

$$L_x = L/x.$$

$$R_\varepsilon = \frac{\varepsilon_2 - \varepsilon_1}{\varepsilon_2 + \varepsilon_1}.$$

THE OLD PROBLEM REVISITED: CHARGES. EFFECTIVE POWER EXPONENT IN A THREE-LAYER SYSTEM





Interaction across the slab

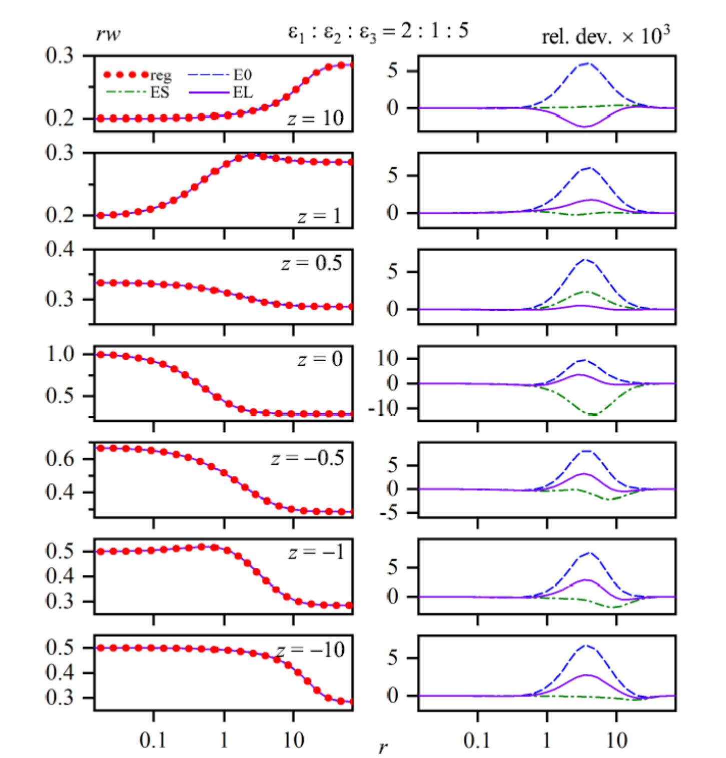
Interaction on the helium film surface

THE OLD PROBLEM REVISITED: CHARGES IN THE SAME LAYER. THREE-LAYER SYSTEM. THE EFFECTIVE EXPONENTIAL APPROXIMATION

$$
\begin{aligned}
w&\left(-\frac{1}{2} \le z = z' \le \frac{1}{2}, r; \varepsilon\right)\\
&\approx \frac{1}{\varepsilon_2}\left[\frac{1}{r} - \frac{\theta}{1+\theta}\frac{1}{\sqrt{r^2 + (2a)^2}}\right]\\
&+ \frac{1}{\varepsilon_2}\frac{\varepsilon_2 - \varepsilon_1}{\varepsilon_2 + \varepsilon_1}\left[\frac{1}{\sqrt{r^2 + (2z+1)^2}}\right.\\
&\left. - \frac{\theta}{1+\theta}\frac{1}{\sqrt{r^2 + [(2z+1) + (2a)]^2}}\right]\\
&+ \frac{1}{\varepsilon_2}\frac{\varepsilon_2 - \varepsilon_3}{\varepsilon_3 + \varepsilon_2}\left[\frac{1}{\sqrt{r^2 + (-2z+1)^2}}\right.\\
&\left. - \frac{\theta}{1+\theta}\frac{1}{\sqrt{r^2 + [(-2z+1) + (2a)]^2}}\right]\\
&+ \frac{1}{\varepsilon_2}\frac{\varepsilon_2 - \varepsilon_1}{\varepsilon_2 + \varepsilon_1}\frac{\varepsilon_2 - \varepsilon_3}{\varepsilon_2 + \varepsilon_3}\left[\frac{1}{\sqrt{r^2 + 2^2}}\right.\\
&\left. - \frac{\theta}{1+\theta}\frac{1}{\sqrt{r^2 + [2 + (2a)]^2}}\right],
\end{aligned}
$$

$$
a = \frac{\theta}{(1+\theta)\ln(1+\theta)}
$$

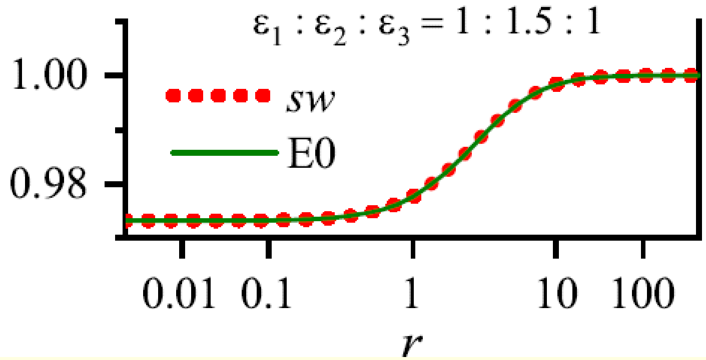
$$
\theta = \frac{\varepsilon_1 - \varepsilon_2}{\varepsilon_1 + \varepsilon_2}\frac{\varepsilon_2 - \varepsilon_3}{\varepsilon_3 + \varepsilon_2}
$$



THE OLD PROBLEM REVISITED: CHARGES INTERACTING ACROSS THE LAYER. THREE-LAYER SYSTEM. THE EFFECTIVE EXPONENTIAL APPROXIMATION

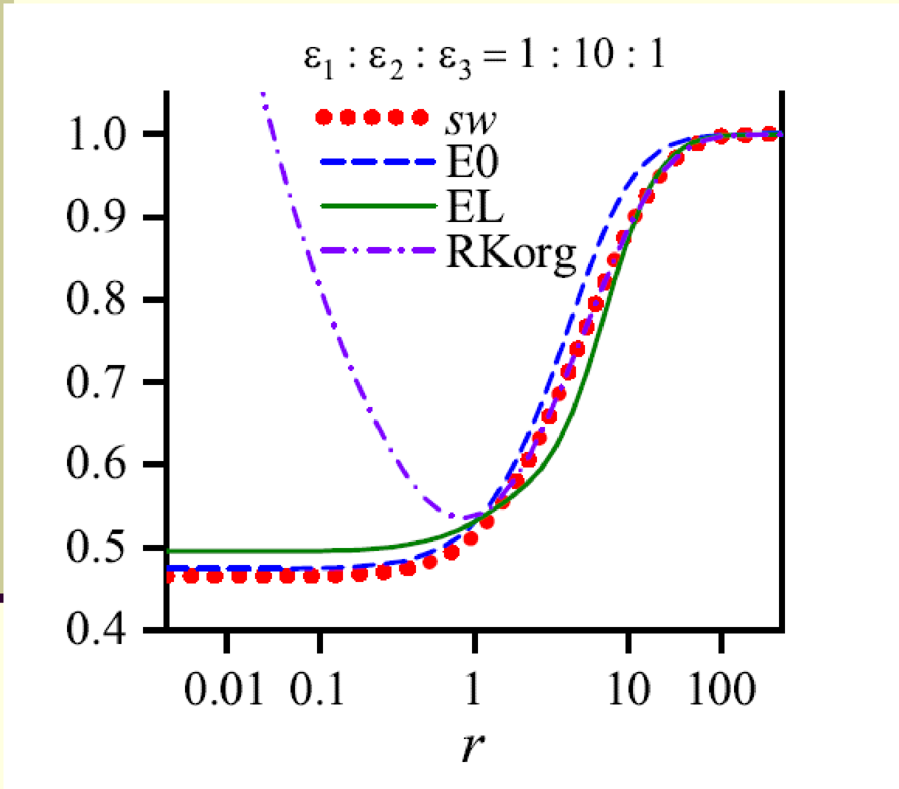
$$w_{13}\left(z=-\frac{1}{2}, z'=\frac{1}{2}, r\right)=\frac{4\varepsilon''}{(\varepsilon'+\varepsilon'')^2}$$
$$\times\left[\frac{1}{\sqrt{r^2+1}}-\frac{\theta}{1+\theta}\frac{1}{\sqrt{r^2+(1+2a)^2}}\right]$$

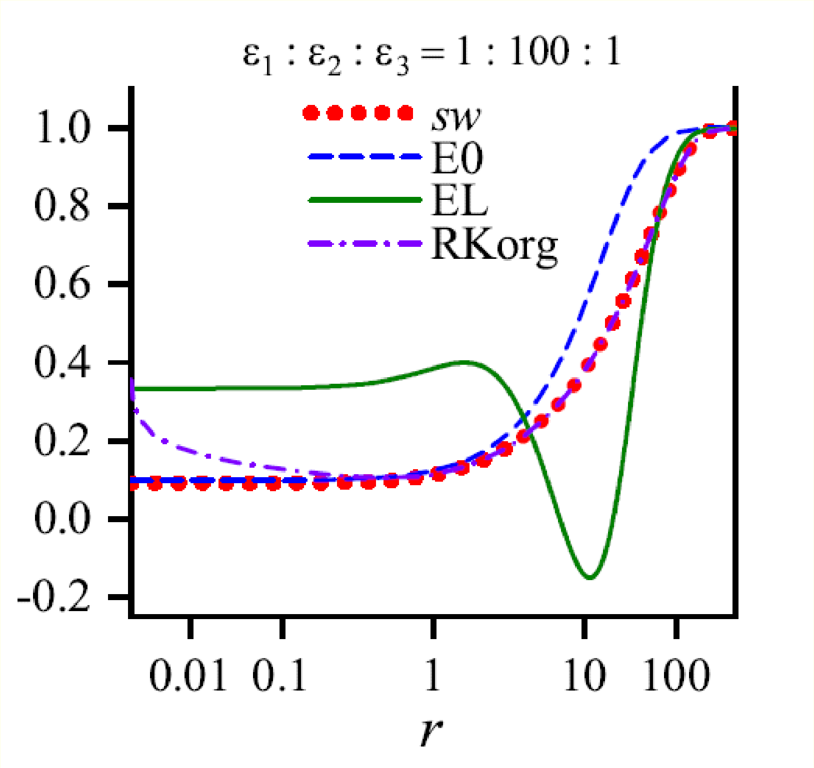
$$\varepsilon_1=\varepsilon_3\equiv\varepsilon'\neq\varepsilon_2=\varepsilon''$$



Dependence $sw(r)$ and its effective-exponential approximation E0 for symmetric structure D

THE OLD PROBLEM REVISITED: CHARGES INTERACTING ACROSS THE LAYER. THREE-LAYER SYSTEM. FAMOUS KELDYSH-RYTOVA APPROXIMATION





THE OLD PROBLEM REVISITED: DIPOLES INTERACTING IN TWO-LAYER SYSTEM. PLANAR ALIGNMENT. CLASSICAL AND INKSON DIELECTRIC FUNTIONS

$$\varepsilon_I(\mathbf{k}) = 1 + \frac{\varepsilon - 1}{1 + \frac{k^2}{\kappa^2}(\varepsilon - 1)}$$

$$W_{PP'}^{\text{cl-cl}}(z = z' = 0) = -\frac{PP'}{L^3(\varepsilon_1 + \varepsilon_2)} \times [\cos(\phi - \phi') + 3\cos(\phi + \phi')], \tag{24}$$

$$W_{PP'}^{\text{cl-In}}(\kappa L \gg 1, z = z' = 0) = W_{PP'}^{\text{cl-cl}}(z = z' = 0) + \frac{3\varepsilon_1(\varepsilon_2 - 1)^3}{(\varepsilon_1 + \varepsilon_2)^2 \kappa^2 L^2} \times [3\cos(\phi - \phi') + 5\cos(\phi + \phi')], \tag{25}$$

$$PP'[\cos(\phi - \phi') + 3\cos(\phi + \phi')] = \mathbf{PP'} - 3\left(\frac{\mathbf{PL}}{L}\right)\left(\frac{\mathbf{P'L}}{L}\right), \tag{27}$$

$$PP'[3\cos(\phi - \phi') + 5\cos(\phi + \phi')] = 2\left[\mathbf{PP'} - 5\left(\frac{\mathbf{PL}}{L}\right)\left(\frac{\mathbf{P'L}}{L}\right)\right]. \tag{28}$$

THE OLD PROBLEM REVISITED: DIPOLES INTERACTING IN TWO-LAYER SYSTEM. NORMAL ALIGNMENT. CLASSICAL AND INKSON DIELECTRIC FUNTIONS

Classical

$$W_{PP'}^{\text{same}}(L, z = z' = 0) = \frac{PP'}{L^3} \frac{2}{(\varepsilon_1 + \varepsilon_2)} \frac{\varepsilon_2}{\varepsilon_1}$$

$$W_{PP'}^{\text{diff}}(L, z = z' = 0) = \frac{PP'}{L^3} \frac{2}{(\varepsilon_1 + \varepsilon_2)}$$

$$W_{PP'}^{\text{In-In,same=diff}}(\kappa_1 L, \kappa_2 L \gg 1, z = z' = 0)$$
$$= \frac{2PP'\varepsilon_1\varepsilon_2}{L^3(\varepsilon_1 + \varepsilon_2)} \times \left\{ 1 - \frac{9\left[\kappa_1 \varepsilon_1^{3/2}(\varepsilon_2 - 1)^{3/2} + \kappa_2 \varepsilon_2^{3/2}(\varepsilon_1 - 1)^{3/2}\right]^2}{L^2\kappa_1^2\kappa_2^2(\varepsilon_1 + \varepsilon_2)^2\varepsilon_1\varepsilon_2} \right\}. \quad (32)$$

It comes about from Eqs. (32)–(34) that the spatial dispersion of dielectric permittivity in the both media or only one of them reduces the dipole-dipole repulsion, which should be taken into account in calculations for dipole lattices [153]. Notwithstanding the smallness of the expansion parameter $1/L^2\kappa_2^2$, the "geometric" coefficient 9 makes the correction factor to the classical asymptotics significant.

CONCLUSIONS

- 1. Coulomb charge-charge interaction is violated due to the appearance of the polarization charges.
- 2. The usage of Rytova-Keldysh formula in exciton physics is sometimes not only inaccurate but totally incorrect.
- 3. A new simple formula is suggested, which is much more simple and accurate than the Rytova-Keldysh one.
- 4. The dipole-dipole interaction is substantially modified by the spatial dispersion of the dielectric permittivity.

PUBLICATIONS

1. A. M. Gabovich, A. I. Voitenko. The 'non-Coulombic' character of classical electrostatic interaction between charges near interfaces // Eur. J. Phys., 2018, v. 39, N 4, 045203 (12 pages)
2. A. M. Gabovich, A. I. Voitenko. Electrostatic interaction near the interface between dielectric media taking into account the nonlocality of the Coulomb field screening // Journal of Molecular Liquids, 2018, v. 267, 166–176